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IRON AND STEEL PRODUCTION

Physicochemical modelling of the classical steelmaking route for life cycle inventory analysis

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Abstract
Goal, scope and background Integrating environmental issues into the traditional product design process, for powerful eco-efficiency, is now one of the major priorities for steelmakers. Life cycle assessment (LCA) is currently undertaken as the most holistic approach for assessing environmental impact and selecting new technologies to reduce emissions for steel industry. However, in order to identify new ways for environmental friendly production of steel, it is essential to carry out the process Life cycle inventory (LCI) which is the core part of LCA. According to LCA practitioners, the quality and the availability of data are the main important limiting factors when applying this methodology for new steelmaking processes without large industrial application. In this paper, we propose a new approach of LCIA of steelmaking, based on the simulation of traditional processes which guarantees the quality of data, the mass and the energy balances. This approach is validated for an existing integrated plant and will be used to assess the inventory for breakthrough steelmaking technologies.

Methods The proposed methodological framework combines physicochemical modelling approach with LCA thinking, in order to carry out the LCI of steelmaking process. Using Aspen Plus commercial flow-sheeting software, physicochemical models have been developed for each steelmaking unit: coke plant, sinter plant, blast furnace, basic oxygen furnace and hot-rolling. The association of the five separately developed modules builds the complete flow sheet of the integrated steelmaking plant. Based on chemical reactions, thermodynamics laws and mathematical equations, the model calculates the mass of each pollutant released by the process, the masses and the chemical compositions of products and by-products simultaneously. For a better understanding of this approach, a brief description of the module developed for coke-making plant is given in the current paper.
Results Thanks to the developed model, the LCI of an existing European integrated steelmaking plant has been calculated and inserted into GaBi software for environmental impacts assessment. In order to check the maturity of the developed approach, simulations of the model have been carried out for virtual cases describing an integrated steelmaking plant, characterised by the best available technology. Comparisons between inventories calculated with the model for “virtual” cases and for existing European plant showed good consistency of results and allowed us to validate the proposed approach.
Discussions The new approach proposed for LCI calculation offers some important benefits that cannot be obtained when the inventory is carried out in the traditional way. First of all, the model allows us to control the mass and energy balances, something that is basically impossible to assure when only data from industry and/or literature are used. Secondly, calculating emissions based on physicochemical and mathematical considerations gives a strong credibility to the inventory. Predictive model simulations,

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for special operating conditions (e.g. recycling of different wastes, use of new fuels or mix of fuels), give access to certain environmental information which is not available. The LCI of the integrated steelmaking plant can then be carried out for different operational practices, and the best scenario can be identified in minimal time.

Conclusions The integrated classical steelmaking route (via blast furnace/converter) has been modelled with Aspen, and the results were successfully compared with industrial data. Consistency of results obtained for simulations of real and virtual integrated plants have shown that the new concept strengthens the LCA method in order to supply rigorous “gate to gate” LCI. It has been shown that the current approach, developed for steelmaking classical route, is mature for modelling new steelmaking breakthrough technologies for environmentally friendly production of steel, such as smelting reduction, direct reduction, hydrogen reduction and use of biomass.

Perspectives After the selection of steelmaking alternatives and before testing these technological proposals at industrial scale, it is crucial to assess their inventories. As perspective of the current work, the approach proposed in this paper can be used as a powerful tool in order to assess the LCI of new technologies mentioned above.

Keywords CO_2 emissions · Integrated steelmaking plant · Inventory data quality · Life cycle assessment · Physicochemical modelling

1 Introduction

During recent years, it was recognised that greenhouse gas emissions (especially CO_2) are the major factor of the global warming effect. In order to meet Kyoto requirements, the steel industry is embracing the challenge of sustainable development by improving its competitiveness and economic success while reducing its environmental impacts. Integrating environmental considerations into the traditional product design process, for powerful eco-efficiency, is now one of the major priorities for steelmakers. However, in order to identify technologies for environmental friendly production of steel, it is necessary to assess the environmental impacts of the current production processes during their life cycles.

Life cycle assessment (LCA) has been undertaken as the most holistic approach for assessing environmental impacts and for selecting new technologies to reduce emissions for the steel industry. The common technical framework for conducting LCA involves the following stages: goal and scope definition, inventory analysis, impact assessment and interpretation of results [Standard ISO 14040 (1997)].

The life cycle inventory (LCI) is the core part of the LCA method which quantifies the relevant inputs and outputs of the steel production system using data collection and calculations.

The quality of the LCA results is dependent on the quality of data used to carry out the LCI (Labouze et al. 1998). Obtaining quality data is important to assure the reliability of the study and to properly interpret the outcomes.

According to LCA specialists, the quality and availability of data used to carry out LCI are the main limiting factors when applying this methodology to steelmaking processes that do not exist yet at large industrial scale. Data used for inventory calculation should respect some essential exigencies, namely the age, the geographical and technological coverage of the data. In many cases, the environmental data related to new steelmaking processes cannot be used due to the lack of measurements of certain pollutants or because the information is much too summarised. It is clear that LCA practitioners are confronted with serious difficulties in respecting these conditions when the LCI is based only on data coming from literature and/or industrial practice. Moreover, it is generally recognised that the classical approach of assessing LCI takes time, and usually, it cannot guarantee the mass and energy balances of flow rates which are considered in the system boundaries.

2 Goal and scope of the study

The objective of our work was to minimise the inefficiency of classical LCIA for new steelmaking breakthrough technologies and to develop a new tool in order to have access in an easier way to environmental information. This new way of carrying out the LCI was validated for the traditional route of steelmaking and guarantees the quality of data, the mass and the energy balances.

The traditional route of steel production is based on the production of hot metal from iron ore, and its conversion to steel in a converter. The proposed methodological framework is based on the interconnection between the environmental tool (LCA) and the process simulation software (Aspen Plus). Advanced system for process engineering (Aspen) is a process engineering software package that is used to simulate processes based on the thermodynamic models, properties of materials and several ready-made unit operation models.

This approach was successfully applied to the classical steelmaking route and has been used in the Ultra-Low CO_2 Steelmaking project (ULCOS) as a powerful tool in the selection of new technologies for environmental friendly steel production. The ULCOS project, under development with 48 partners from 14 European countries, is one of the

most ambitious European projects aimed at developing new technologies for reducing steelmaking emissions, compared with the iron ore-based benchmark.

Based on the proposed approach, the LCI has been carried out for the classical route of steel production. In terms of system boundaries, the study covers the foreground processes: coking plant, sintering plant, blast furnace, converter (or basic oxygen furnace), continuous casting and hot-rolling. The interconnection of these processes is given in Fig. 1.

The electricity required to operate the process was also considered in the system boundaries. It was assumed that an internal power generation plant, which uses steelworks gases (namely, blast furnace gas, coke oven gas and basic oxygen furnace gas), supplies the electricity. For the first stage of our study, the system considered does not include the extraction of raw materials, their transportation to the plant and the waste storage.

In order to ensure the comparability of LCA results, the selected functional unit (FU) for the current study is 1 t of hot-rolled coil produced in a classical integrated steelmaking plant.

3 New methodological framework proposal

As already mentioned, the new methodology proposed in this paper consists of the interconnection of the LCA method with process physicochemical modelling as illustrated in Fig. 2.

Hence, the LCI is carried out with simplified physicochemical models developed for each process of the integrated steelmaking plant as defined by the system boundaries. These processes have been modelled using Aspen Plus commercial simulation software equipped with a thermodynamic database, which is used to design process flow sheets and to calculate mass and heat balances.

Basically, the major part of the LCI data is supplied by the results of the Aspen models and completed in some instances by measured data (e.g. uncontrolled emissions).

Thanks to Aspen's modular structure, chemical reactions, thermodynamics laws and mathematical equations were all taken into account for modelling each defined process. Finally, the association of the five separately developed modules builds the complete flow sheet of the integrated steelmaking plant.

These modules calculate the mass and heat balances, air emissions and the chemical compositions of products and by-products simultaneously. The quality of the products and by-products obtained by model simulation is given by their chemical compositions, which are checked constantly and attentively.

The new approach offers some important benefits that cannot be obtained when the LCI is carried out in the traditional way, using data only from industry and/or literature.

First of all, the model allows us to control the mass and energy balances of the calculated inventory, something that is nearly impossible to assure when the LCI is carried out in the traditional way. Secondly, calculating air emissions based on physicochemical and mathematical considerations gives a strong credibility to the inventory and in consequence of this, the precision of data is guaranteed. Finally, model simulations for special operating conditions, such as recycling of different wastes, the use of new fuels or the mixing of fuels, give access to certain environmental information which is not available among the industrial or literature outputs. In this way, the representativeness and the reproducibility of data are assured. Based on the proposed approach, the LCI of the integrated steel plant can be carried out for different operational practices and the selection of the best operational scenario, from environmental point of view, can be done in minimal time.

Due to the complexity of steelmaking processes and for clarity reasons, the description of the integrated model developed in the frame of our work is skipped in this paper. Full details about the model and about the simulations which allowed its validation with industrial data are given elsewhere (Iosif et al. 2008a, b; Iosif 2006). However, an overview of the main inputs and outputs of the global model is given below for each process. Coking model

(a) Input data: energy for the coke oven heating, mass and elementary composition of mix coals, average composition of tar and final temperature of coking products.

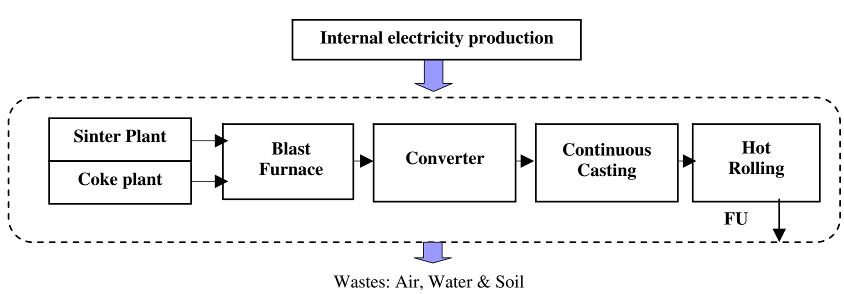

Fig. 1 Steelmaking system boundaries

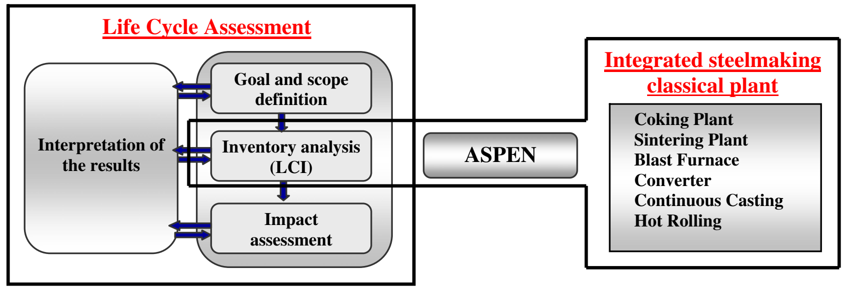

Fig. 2 New methodological framework for LCI analysis

(b) Output data: flow rate and composition of coke oven gas, mass and composition of coke, tar and light oils masses, water of carbonization mass, ammonium sulphate mass and waste gas composition for coke oven heating.

Sintering model

(c) Input data: energy for ignition, mass and chemical composition of raw materials, sinter Fe^{2+} content, oxygen content into the fumes and efficiency of waste gas cleaning facilities.

(d) Output data: sinter mass and composition, sintering fumes environmental burden: volume of fumes, CO_2, CO, SO_2, NO_2, VOC, heavy metals (Pb, Cd, Hg), HCl and dust emissions

Blast furnace model

(e) Input data: mass, chemical composition and final temperature of hot metal, mass and chemical composition of some raw materials, heat loses into the throat and bosh zones and energy requested for blast heating.

(f) Output data: mass of requested sinter, mass of consumed coke, volume and composition of blast furnace gas, mass and composition of slag, steelmaking gas consumption and waste gas composition for blast heating.

Converter Model

(g) Input data: mass and chemical composition of raw materials, mass and composition of liquid steel.

(h) Output data: mass and composition of converter gas, mass and composition of slag, mass and composition of dust, volume of oxygen needed and thermal losses.

4 Life cycle inventory assessment using Aspen model

Using the global model and industrial data, the LCI of an existing European integrated steelmaking plant has been successfully calculated. The inventory calculated by the model has been inserted into GaBi software in order to assess the environmental impacts for the analysed case. GaBi allows us to quantify emissions which are not calculated by the model (i.e. uncontrolled emissions). As illustration, a part of the LCI calculated with the model for the given European integrated plant is summarised in Table 1.

5 Validation of the new approach for LCI assessment

In order to check the maturity of the developed approach, two Aspen simulations have been carried out using:

(a) industrial data supplied by a European integrated steelmaking plant,

(b) "benchmark" data supplied by the ULCOS project. In the frame of the ULCOS project, the "benchmark" data defined an integrated steelmaking plant characterised by the best available technologies.

The inventories calculated by the model for both cases have been compared between them and to one another, considered as a reference LCI. This reference LCI has been developed by the International Iron and Steel Institute (IISI; IISI World Steel Life Cycle Inventory 2000) to quantify the use of resources, energy and environmental emissions associated with the processing of 14 worldwide steel plants. For all three cases, LCI are reported at the same functional unit derived via the blast furnace/basic oxygen furnace route. The comparison between these three "gate to gate" LCI has been possible thanks to GaBi software. The objective of this comparison was to demonstrate the maturity of the model for given reliable inventories of real cases such as the integrated European plant but also of "virtual" cases such as the ULCOS benchmark. As illustration, in the current paper, it was preferable to show only the comparison of CO_2 emissions between the three scenarios. This comparison is outlined in Fig. 3. Hence, total CO_2 emission released by the defined processes is 1,147 kg/FU (European integrated plant), 937 kg/FU (ULCOS benchmark) and 1165 kg/FU (IISI reference case).

In this figure, the CO_2 emissions are calculated for each process without taking into consideration the consumption of electricity. CO_2 variance between the analysed cases is basically linked to the difference masses of raw and

Table 1 Summary of the integrated steelmaking plant inventory calculated by the model

Flux	Identification	Unit	Quantity
Materials inputs	Iron ore	kg/FU	1,321
	Coal for coke-making	kg/FU	430
	BF injection coal	kg/FU	154
	Scraps	kg/FU	127
	Pellets	kg/FU	139
	Lime	kg/FU	40
Energy inputs	Internal electricity	MJe/FU	884
Intermediates products	Sinter	kg/FU	1,403
	Coke	kg/FU	336
	Hot metal	kg/FU	1,020
	Liquid steel	kg/FU	1,077
	Slabs/blooms	kg/FU	1,027
	Coke oven gas	Nm^3/FU	132
	Blast furnace gas	Nm^3/FU	1,478
	Converter gas	Nm^3/FU	82
Material outputs (by-products)	Slag	kg/FU	423
	Tar	kg/FU	10
	Ammonium sulphate	kg/FU	4
Product	Hot-rolled coil	kg/FU	1,000
Emissions to air	CO_2[a]	kg/FU	1,587
Emissions to land	Sintering dust	kg/FU	1

[a] "gate to gate" system boundaries according to Fig. 1

intermediate materials (coke, sinter, hot metal...) used in the process. Moreover, the use of various types of fuels for heat supply (blast furnace, coke oven, converter gas and natural gases) can also contribute to the variation of emission due to the chemical composition and the heat capacity of these gases.

As mentioned, the system electricity is supplied by internal production using steelworks gases, namely blast furnace gas, coke oven gas and converter gas, which are considered as by-products of coke, hot metal and steel. It is important to stress that the entire amount of steelworks gases produced in the system is not consumed only for electricity generation. In reality, prior to electricity production, some of the gases are used in the system as heat supply for coke oven heating, hot-rolling stoves and blast stoves as indicated in Fig. 4.

A schematic representation of the steelworks gases used in an integrated plant is given in Fig. 5.

The difference between the production of these gases and their consumption as heat supply is called “excess of steelworks gases”. This excess is used mainly for internal electricity production but also as an energy supply for auxiliary facilities such as raw materials preparation, lime production and steam production. For the current LCA study, these facilities are not considered in the system boundaries.

The production of electricity using steelworks gases was also simulated with a simplified Aspen module developed

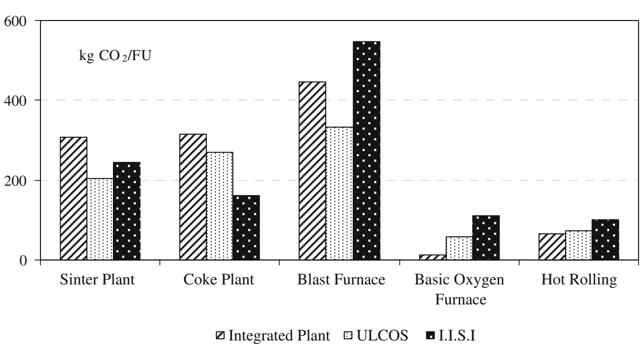

Fig. 3 Inventory of CO_2 emissions for each steelmaking process included in the analysed system

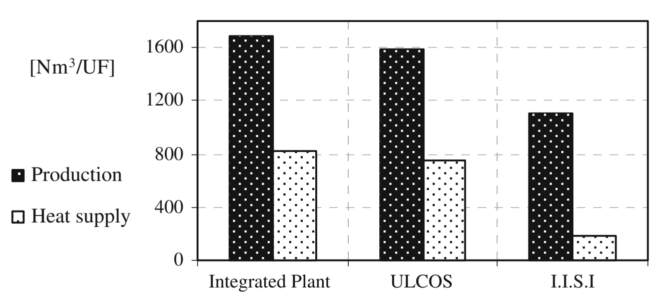

Fig. 4 Steelworks gases production and internal consumption as heat supply

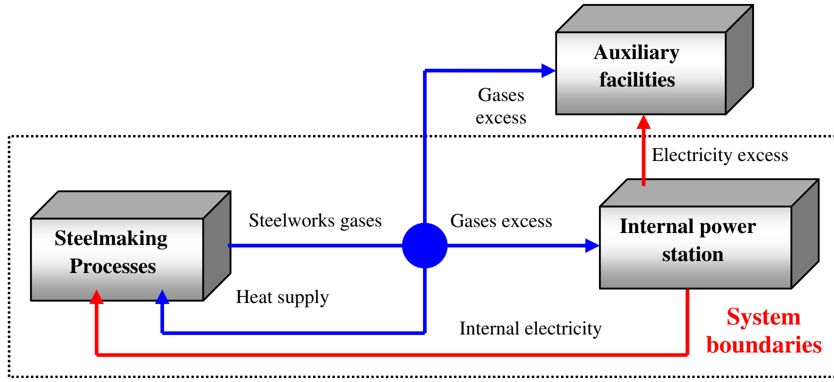

Fig. 5 Internal electricity production

for an internal power station. The CO_2 emissions calculated with this module for the production of electricity required by the system are given in Table 2.

Table 2 also sums the amount of CO_2 released by the production of 1 t of hot-rolled coil as defined by the system boundaries. As can be seen in the table, the CO_2 emissions for the ULCOS benchmark are less significant because this scenario is based on the consumption of a large amount of pellets in the blast furnace. The environmental burden of pellet production is lower than the burden of sinter production. In addition, in the ULCOS scenario, the coal injection in the blast furnace reaches the maximum rate, and consequently, the consumption of coke is reduced. Indeed, the decrease of coke demand leads to lower environmental burden for the system. The CO_2 emissions calculated by the model for the European steelmaking plant were successfully compared with the average value of 14 plants derived from the IISI inventory. This result emphasises the maturity of the model and fortifies the reliability of the proposed approach.

According to the steel people, the industrial experience shows that there is no excess of energy when all the auxiliary facilities (raw materials preparation, lime production, steam production) are part of integrated plant. If the system boundaries are extended towards auxiliary facilities, the environmental burden involved in the total consumption of steelworks gases in the frame of the system should be integrated into the LCA study (see Table 2 for CO_2 emissions). Thanks to the current approach, it has been shown that by using the best available techniques and optimising the use of resources, the environmental burden can be notably reduced. To exemplify, the CO_2 emissions can be reduced by 200 kg of CO_2/FU for the ULCOS benchmark case. Finally, it is important to stress that the agreement between results obtained for the ULCOS benchmark and the European plant cases validates of the current approach.

Table 2 CO_2 emissions involved in the integrated steelmaking plant

CO_2 emission [kg/FU]	Integrated plant	ULCOS	IISI
Steelmaking processes	1,147	937	1,165
Electricity production	440	510	499
System total emissions	1,587	1,447	1,664
Auxiliary facilities	362	293	344
Total	1,949	1,740	2,007

The consistency of results for the simulation of a “virtual case” represented by the ULCOS benchmark shows that the new concept is now mature enough to model “new routes” for steel production, which are investigated under the ULCOS umbrella.

6 Conclusions

In the present paper, we have proposed and developed a new methodological framework which combines a physicochemical modelling approach with LCA thinking, in order to carry out the LCI of steelmaking processes.

The integrated classical steelmaking route (via blast furnace/converter) has been modelled with Aspen software and the results were successfully compared with industrial data. It was shown that the validated model is a powerful tool in order to provide a rigorous “gate to gate” inventory. Moreover, the model allows the calculation of the chemical compositions of products and by-products such as the steelworks gases. This information is very important because the steelworks gases are used as fuels by all of the steelmaking processes. Hence, the contribution of these gases to the total environmental burden of the system can be easily estimated. Also, the developed model helps different companies rapidly assess their environmental impacts with respect to their own industrial configuration.

The main advantages offered by this new methodology framework for LCI assessment are the ability to predict

emissions for different flow sheets and to control the mass and the heat balances of the analysed process. Consequently, the quality of data used in LCI is automatically guaranteed. Moreover, the environmental burden for special conditions such as gas and waste recycling can be rapidly calculated, and the best scenario for each processing route can be easily selected. These attributes give a strong credibility to the calculated inventory and allow LCI analysis to proceed more quickly.

In the present work, it was proved that the current approach is mature for modelling breakthrough steelmaking technologies such as smelting reduction, direct reduction, hydrogen reduction and use of biomass for environmentally friendly production of steel. Indeed, after the selection of new steelmaking alternatives and before testing these technological proposals at industrial scale, it is crucial to assess their inventories. Hereafter, the approach proposed in this paper can be used as a powerful tool in order to assess the LCI of new technologies selected in the frame of the ULCOS project.

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